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Boundary conditions for dislocation dynamics simulations and stage 0 of BCC metals at low temperature

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ABSTRACT

In order to study the dislocation density evolution of body centered cubic (bcc) crystals at low temperature by dislocation dynamics (DD) simulations, we investigated carefully three different boundary conditions (BC) for DD, i.e., the quasi-free surface BC, the flux-balanced BC, and the periodic BC. The latter two BCs can account for the dislocation loss from the boundary of the finite simulation box. PBC can also eliminate the influence of surfaces and improve the line connectivity. We have found that the PBC provides a convenient and effective boundary condition for DD simulations and have applied it to the study of dislocation density evolution of bcc metals during stage 0 deformation at low temperature.

INTRODUCTION

At low temperature, the plastic deformation of bcc metals is dominated by the low mobility of the screw dislocations that move by a thermally activated kink pair mechanism. In contrast, the edge dislocations practically see no lattice friction and are extremely mobile. The strong anisotropy in the dislocation mobility of the screw and edge has certain direct consequences on the mechanical properties of bcc metals at low temperature. First, the macro-yield stress is determined by the kink pair mechanism and critically depends on the kink pair activation enthalpy [1]. Second, in contrast with the usual behavior, the well established relation between the flow stress and the square root of the dislocation density breaks down [2]. Third, there exists a so-called stage 0 before macro-yield where the plastic deformation is mainly carried out by edge dislocation motion [3]. During this stage, the dislocation density increases significantly. Thus, unlike what is usually assumed, the dislocation density at yield can be substantially larger than the initial density.

Our objective is to study the strain hardening of bcc metals at low temperature using DD simulations. In previous work, we have simulated the yield stress and the forest hardening quantitatively using single crystal tantalum as a model material. In this work, we present preliminary results on the dislocation density evolution during stage 0 of the plastic deformation. An essential step towards a realistic simulation consists of implementing a proper boundary condition for the DD simulations that allow realistic dislocation density increase and plastic strain during stage 0 to be reached. In this paper, we first present the three boundary conditions implemented in the DD simulations and discuss their strengths and weaknesses. We then present results on the dislocation density evolution during stage 0 at different temperatures using PBC. Finally, some discussions and conclusions are presented.

BOUNDARY CONDITIONS

Due to significant differences between the dimensions of bulk specimens and simulated volumes, the existence of simulation box surfaces can create artifacts. Dislocations disappear from the box by reaching the outer surfaces, which can lead to significant density losses. The situation is particularly serious for bcc metals at low temperature because edge dislocations have very large mean free path relative to the slow screws. In the following, we review three types of boundary conditions implemented in our DD simulation and discuss their effects on the simulated mechanical properties.

Quasi-free surface BC

During the early development of DD simulations, a quasi-free surface boundary condition (QBC) was used [4]. As schematically shown in figure 1(a) a DD simulation is performed inside the cubic simulation box, where dislocations moving out of the simulation box simply disappear. This causes a depletion of the density close to the surfaces. To minimize the effect of the surfaces, a sphere embedded in the cube is considered so that only dislocations inside the sphere are tracked for the calculation of strain and density. The sphere is chosen so that within it the dislocation density is more or less uniform. For bcc metals at low temperature, this method was found to be ineffective. Due to the strong mobility difference between edges and screws, the fast moving edges can reach and leave the box surfaces easily, leaving behind long screw dislocation segments. The dislocation microstructure is typically rather uniform and there is no apparent improvement by using the sphere method.

Flux-balanced BC

The flux-balanced BC (FBC) is based on a continuum mechanical frame and was initially proposed by El-Azab [5]. It provides a statistical means to account for the dislocation loss from the simulation box. It states that a representative simulation box should maintain balanced net dislocation flux for each slip system. Or, the sum of outward areas swept by all dislocations in each slip system should be equal to the inward swept area, as shown schematically in figure 1(b). To implement this flux balance in the DD simulation, an inward flux is purposely introduced at the boundaries in the form of half loops. These half loops propagate into the simulation box and contribute to the plastic flow. This method was implemented in our DD code and was found to increase both the plastic strain and dislocation density significantly during stage 0 plastic deformation of bcc metals at low temperature [6].

However, there are some drawbacks associated with this method when applied to a DD simulation. The implementation is complex since it requires the calculation of the swept area by each individual dislocation segment and to deal with a variety of shapes as illustrated by figure 1(b). Another difficulty is that the half loops introduced can not be arbitrary since they have to

meet a critical size requirement to avoid immediate disappearance due to the line tension forces. This critical size has to be stress dependent. As a result, the smallest increment of the inward

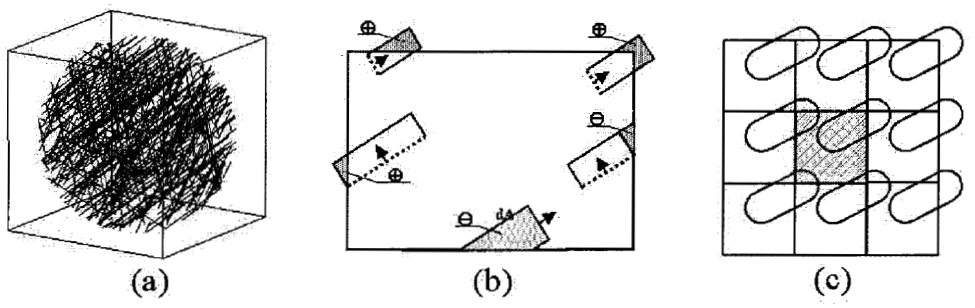

Figure 1. Schematic drawing of the three boundary conditions. (a) is the quasi-free surface BC; (b) is the flux-balanced BC where the shaded areas show the outward (plus sign) and inward (minus sign) 'swept-areas'. **dA** represents a half-loop of critical size that has been introduced; (c) depicts the periodic BC, where the shaded central area shows the primary simulation box.

swept area should be equal to the size of one critical half loop at a given stress state. This means that the outward flux can not be instantaneously balanced by the inward flux. If the outward flux is smaller than the size of a critical half loop, it should be accumulated and balanced by introducing an inward loop at a later time when the stress or strain is larger. This inability of the FBC to maintain the detailed balance of inward and outward flux shows itself during stage 0, giving rise to a delayed effect that may cause overestimated slip activity.

Periodic BC

PBC has been a standard method to mimic an infinite system by translational repetitions of a small representative volume of material. Though it is a common practice for particle systems, it is not transparent that the method can work for three-dimensional dislocation networks. Bulatov et al. [7] recently implemented PBC for three-dimensional DD simulations that shows certain potential advantages. The numerical implementation is very simple. Similar to particle systems, the algorithm involves arithmetic manipulation of *modulo periodicity vectors*, i.e.,

$$dx_i = dx_i - l_i \cdot \mathrm{nint}(dx_i / l_i), \quad i = 1, 2, 3 \qquad (1)$$

where dx_i is the distance between two points along Cartesian direction i, l_i is the corresponding primary box length, and nint is the modulo operation. A two dimensional schematic representation of a PBC system for dislocations is shown in figure 1 (c), where the shaded box is the primary simulation box which is surrounded by its images. Contrary to what is discussed in [7], the initial configuration compatibility issue practically proposes no constraint at all. The advantage of the PBC is that it eliminates the influence of surfaces since no segment ends at the simulation box surfaces. This is an improvement compared to QBC and FBC discussed earlier where the intersection of segments with surfaces could not be treated properly. In this regard, PBCs provide better accuracy in overall line tension calculations and this manifests in dramatically decreased fluctuations in the simulated stress-strain curves. In addition, unlike

FBC, the dislocation density is instantaneously balanced in the primary simulation box. As a result, we have observed almost identical contributions to plastic strain from the screw and edge dislocations at the end of stage 0, where both QBC and FBC show that the screw dislocations contribute significantly more compared to the edges.

Despite the advantages the PBC provides, a dislocation system with PBC does not represent an infinite one. The primary simulation box size needs to be large enough to contain the characteristic physical length scale of the dislocation microstructure studied. All the simulation box sizes presented in this work are 15μm or larger. In addition, a correlation effect related to the choice of the simulation box shape could potentially affect simulation results. To illustrate this point, figure 2 schematically shows a cross section of the areal glide of a pair of anti-parallel dislocations in the same loop and in two different boxes. In the case of a cubic box shown in (a), the dislocation line is found to annihilate with its own loop after translation by one replica of the primary box. In the case of a non-cubic (e.g., orthorhombic) box, the dislocation can form strong dipoles with part of its own loop after a few translations of replicas, depending on the shape of the box. A cubic box presents the strongest correlation and should be avoided. Although there is no unique choice of non-cubic box shapes, it is preferred to have incommensurate numbers between the three Cartesian box lengths.

In order to check the sensitivity of the simulation results to the box shape, we have performed identical simulations using three different orthorhombic simulation boxes. The results are shown in figure 3. Essentially, one is unable to tell the difference between the three, which is certainly good for the practical use of PBCs. But this is unexpected since the schematic drawings in figure 2 would predict differently. The reason is that, before the strong self-correlation effect similar to figure 2 occurs, all simulations should statistically behave in the same manner. It takes a certain minimum strain for a free gliding single dislocation to reach the point where it interacts with its own image. In a practical simulation with many dislocations and with forest hardening, that minimum strain is rather large. A simple estimate using typical dislocation density and simulation box size (as those in figure 3) shows that the correlation effect will not occur until a plastic strain in the order of 1%, which is much larger than the plastic strain reached in the present simulations. In addition, with forest hardening and other dislocation interactions, this minimum strain value will further increase significantly. Therefore, for the purpose of our study of the stage 0, the choice of the simulation box shape does not propose a problem. In the following, we will use PBCs to perform DD simulations of stage 0 deformation.

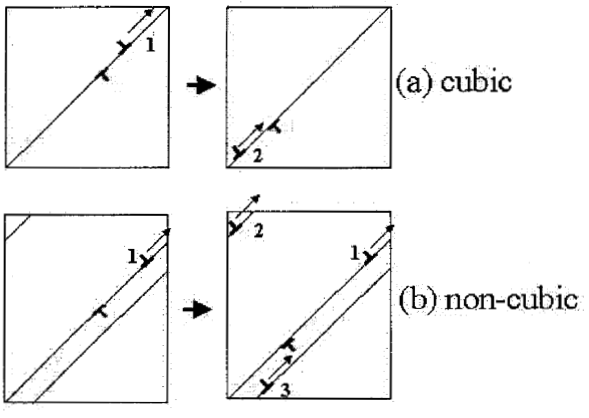

Figure 2. Schematic drawings to show the correlation behavior for different choices of simulation box shapes, i.e., a cubic box (a) vs. a non-cubic one (b). An initial pair of anti-parallel dislocations in the same loop is moving in its primary slip plane (left). At a later time, one of the initial dislocations moves out and its image segment enters into the primary box (right). The image segment can annihilate (in (a)) or form a dipole (in (b)) with the second primary dislocation.

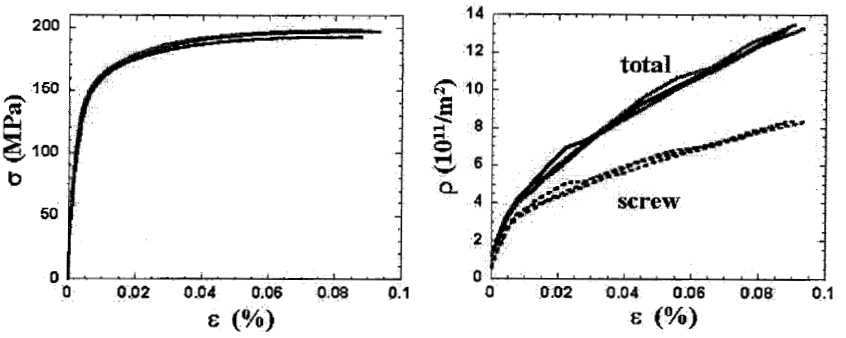

Figure 3. Simulated stress-strain curves (left) and dislocation density (right) for a $\bar{4}819$ tantalum crystal for 3 orthorhombic simulation boxes. The box lengths of the three sides are (6168, 6768, 7362), (6168, 6174, 6180), and (6168, 6666,7460) respectively (6168 corresponds to 15μm). The simulations are performed at 215K and at 10^{-3}/s strain rate. The initial dislocation density is $10^{11}/m^2$ with equal amount of screw and edge randomly distributed around an average length of 5μm. For more detail on the DD simulation, see [1].

RESULTS OF DISLOCATION DENSITY EVOLUTION

Stage 0 plastic deformation of bcc single crystals at low temperature is defined as the plastic deformation before macro-yield and is mainly carried out by edge dislocations. Experimentally, it is found that during stage 0, the dislocation density can increase significantly. Since the subsequent forest hardening depends strongly on the dislocation density [2], it is imperative to understand and simulate quantitatively the dislocation density evolution during stage 0. Figure 4 shows the simulated stress-strain curves and the dislocation densities at different temperatures. One can see that the lower the temperature, the higher the flow stress is. This is due to the thermally activated character of screw dislocation mobility [1]. Also, the lower the temperature, the higher the total and screw dislocation densities are at the end of stage 0. Initially, the simulation contains a population of edge segments with different lengths that are activated at different stress values. Since the main mechanism for dislocation density increase during stage 0 is by the motion of edge dislocations trailing long sessile screw segments, a higher stress activates shorter edge segments and more edge dislocations contribute to plastic flow. Thus, it generates more elongated screw dislocations. This explains the observed higher screw dislocation density at lower temperature. It's worthy to point out a difference between using PBC and the previous two BCs. There are continuous slip activities of edges throughout stage 0 by the PBC. For the previous two BCs, the edge segments were seen to be almost completely exhausted before the macro-yield was reached.

CONCLUSION

We have implemented three boundary conditions for DD simulations. Both FBC and PBC provide means to balance in and out dislocation fluxes at the surfaces of the simulation box.

FBC balances dislocation flux in a global way since it does not balance each detailed dislocation loss. For a small system with low dislocation density, the balance is likely to involve a time delay.

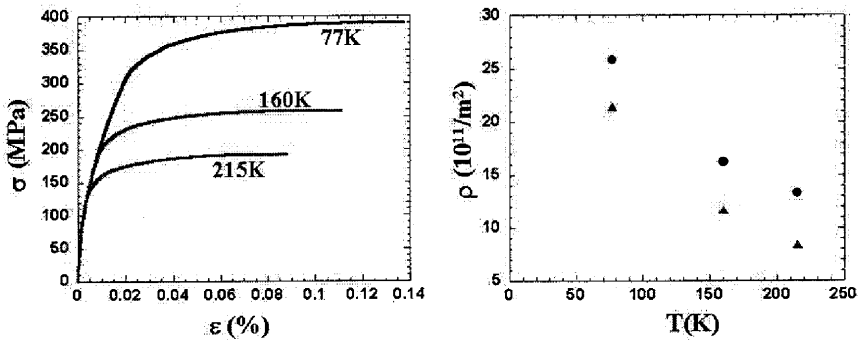

Figure 4 Simulated stress-strain curves (left) and dislocation density (circles for total density and triangles for screw density) vs. temperature (right) for tantalum during stage 0. The initial configuration and numerical conditions are the same as in figure 3.

PBC provides detailed instantaneous balance of dislocations out of the primary box. In addition, PBC eliminates the existence of surfaces and the related difficulties. Although the choice of different simulation box shapes could impose an intrinsic problem for PBC since the simulation results may not be unique, our simulation results show that this is not a problem in practice. We have applied a DD simulation with PBC to simulate the low temperature stage 0 of bcc metals. Our first results show that the plastic strain at the end of stage 0 is in the order of 0.1% and the total dislocation density has increased by at least one order of magnitude. These values are similar to those suggested by experimental data [3]. In the future, our DD simulations with PBC will be used to analyze in detail the density evolution during stage 0 for bcc metals. Our objective is to develop a phenomenological model to understand the density evolution as a function of the strain rate, temperature and initial dislocation configurations.

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